Vortex induced deformation of the superconductor crystal lattice

Pavel Lipavský[1], Klaus Morawetz[2,3], Jan Koláček[4] and Ernst Helmut Brandt[5]
[1] *Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic*
[2] *Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany*
[3] *Max-Planck-Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany*
[4] *Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic and*
[5] *Max-Planck-Institute for Metals Research, D-70506 Stuttgart, Germany*

Deformation of the superconductor crystal lattice caused by Abrikosov vortices is formulated as a response of the elastic crystal lattice to electrostatic forces. It is shown that the lattice compression is linearly proportional to the electrostatic potential known as the Bernoulli potential. Eventual consequences of the crystal lattice deformation on the effective vortex mass are discussed.

PACS numbers: 74.25.Fy, 74.25.Ld, 74.25.Qt, ,74.81.-g, 78.20.-e,

During the transition from a normal to a superconducting state, metals reduce their specific volumes [1, 2]. In a mixed state, would it be the Abrikosov vortex lattice or a structure of lamellas, the superconductivity is locally suppressed and the specific volume is inhomogeneous. The mixed state is thus accompanied by strains and stresses, which enter the balance of total energy.

In general, the energy of strains is much smaller than the energy of the superconducting condensation and the energy of the magnetic field. Its contribution becomes appreciable only under special conditions. For example, experiments on single crystals of Pb-alloys [3, 4] and Nb-alloys [4, 5, 6] revealed that an orientation of the vortex lattice is influenced by its angles to main crystal axes. Since the gap of alloyed samples is quite isotropic, purely electronic models have failed and this effect has been explained with the help of strains induced by vortices [7].

In the 1990th a different structural effect has been observed on $NbSe_2$. If the magnetic field is tilted from the *c*-axes, the Ginzburg-Landau (GL) theory predicts a state in which rows of vortices are aligned with the direction of tilting [8], while experiments [9, 10, 11, 12] show them aligned in the perpendicular direction. Again, the interaction of vortices with the crystal strain explains the observed alignment [13].

Finally, we would like to mention phenomena which are predicted but not yet fully experimentally confirmed. Perhaps, one of the most interesting predictions is a sizable contribution of the lattice deformation to the mass of vortex [14, 15, 16, 17]. Besides, there is a number of phenomena due to strains at surfaces which are discussed in Ref. [18]. It is also argued that the strain can mediate an attractive long-range interaction between vortices [19].

As far as we know, all theoretical studies of deformable superconductors use a phenomenological model, which assumes that the superconducting condensate interacts with the lattice density directly via a strain dependence of material parameters. This model dates back to the 1960th [20, 21], when it was used to describe the vortex pinning. The strength of the interaction is deduced from changes of the specific volume in the phase transition, see also Ref. [14].

In this paper we assume that the condensate interacts with the crystal lattice via electrostatic forces created by the so called Bernoulli potential. We show that this mechanism results in the interaction based on the specific volume. In addition to known theories we obtain gradient corrections and demonstrate that they are important for the vortex motion of the Abrikosov vortex lattice in niobium.

In an isotropic continuum, the displacement field $\mathbf{u}$ obeys the equation [22]

$$\left(K+\frac{4}{3}\mu\right)\nabla(\nabla.\mathbf{u})-\mu\nabla\times\nabla\times\mathbf{u}=\mathbf{F}, \qquad (1)$$

where K and μ are the bulk and shear modulus, and $\mathbf{F}$ is the volume density of force acting on the lattice. Some authors prefer to express coefficients on the left hand side in terms of the Poisson ratio $\sigma=(3K-2\mu)/(6K+2\mu)$ and the Yang modulus $E=3K(1-2\sigma)$. In the basic approximation K and μ are constants. Their small change in the superconducting state was assumed in [23].

The inhomogeneous superconductivity results in the force $\mathbf{F}$. The present theory differs from previous approaches in the approximation adopted for $\mathbf{F}$. Let us sketch the approach based on the specific volume first. More details the reader can find in Ref. [15].

In the phase transition from the normal to the superconducting state, a system shrinks by a volume difference $\delta V=V_{\rm n}-V_{\rm s}=\alpha_T V$. A typical value of α_T is about 10^{-7}. The density of the atomic lattice correspondingly increases, $\delta n_{\rm lat}=n_{\rm lat}^{\rm s}-n_{\rm lat}^{\rm n}=\alpha_T n$.

The strain coefficient α_T depends on the temperature via a fraction ω of electrons, which become superconducting, $\alpha_T=\alpha\omega$. Here α is the strain coefficient at zero temperature. In the spirit of the GL theory, we express the superconducting fraction in terms of the GL function $\omega=2|\psi|^2/n$, i.e., $\delta n_{\rm lat}=2\alpha\,|\psi|^2$.

In the vortex core or in the region of surface currents, the GL wave function changes in space, see Fig. 1. The lattice then tends to be inhomogeneous, which causes

internal stresses. These stresses lead to a density of force

$$\mathbf{F}_{\rm Sim} = K\,\alpha\,\nabla\frac{2|\psi|^2}{n} \qquad (2)$$

proposed by Duan and Šimánek [15] in their study of the vortex mass. The phenomenological formula (2) furnishes us with a density of forces with no regards to how the superconducting electrons are coupled to the lattice.

Let us try to express such force on the lattice in a semi-microscopic way. Diamagnetic currents, either being on the surface or circulating around the vortex core, always cause inertial and Lorentz forces, which are balanced by an electrostatic field $\mathbf{E} = -\nabla\phi$, see London [24]. This electric field transfers the Lorentz force from electrons to the lattice, therefore one can expect that it also causes lattice deformations. Accordingly, we suppose that the electrostatic field force

$$\mathbf{F} = en\,\nabla\phi, \qquad (3)$$

is playing the role of the force $\mathbf{F}$ in equation (1). For simplicity of notation we assume singly ionized atoms, e is the charge of an electron, so that the ionic charge density is $-en$.

The electrostatic potential ϕ is known as the Bernoulli potential. It has been derived in a number of approximations [24, 25, 26, 27]. Here we will use the formula of Ref. [27]

$$\begin{aligned} e\phi \;&=\; -\frac{1}{2m^*n}\bar\psi\left(-i\hbar\nabla - e^*\mathbf{A}\right)^2\psi \\ &+\; \frac{\partial\varepsilon_{\rm con}}{\partial n}\frac{2|\psi|^2}{n} + \frac{T^2}{2}\frac{\partial\gamma}{\partial n}\left(\sqrt{1-\frac{2|\psi|^2}{n}}-1\right). \end{aligned} \qquad (4)$$

The space profile of the potential ϕ is shown in Fig. 2 and the individual terms to the potential are compared in Fig. 3. The first term in (4) is the quantum kinetic energy and represents the gradient corrections. In the London limit it reaches the form of the classical Bernoulli law, $\bar\psi\left(-i\hbar\nabla - e^*\mathbf{A}\right)^2\psi/2m^*n \;\rightarrow\; e^{*2}A^2\omega/4m^* = \omega m v^2/2$, which gave the name to the entire potential. The superconducting fraction ω multiplying the kinetic energy accounts for the fact that the Lorentz and inertial forces act exclusively on the super-electrons, while the balancing electrostatic force acts on all electrons [25]. This force being proportional to the square of the magnetic field has been used to calculate the shape distortion by flux-pinning-induced magnetostriction [28].

The second term of the Bernoulli potential (4) is the dominant one and we will focus our discussion on it. This second term is identical to the potential derived by Khomskii and Kusmartsev [26] from the effect of the BCS gap on the local density of electronic states. The third term of (4) we call the entropic correction.

It is worth noting that all the three equations (4), (3) and (1) are resulting from Gibbs variational principle if the free energy used in [27] is extended by the ionic lattice deformation energy.

Let us link the deformation caused by the electrostatic field with the standard theory of magnetostriction. At zero temperature, the Gibbs energy of normal and superconducting states differ by the condensation energy [2], $G_{\rm s} = G_{\rm n} - V\varepsilon_{\rm con}$, where $\varepsilon_{\rm con} = \gamma T_{\rm c}^2/4 = B_{\rm c}^2/2\mu_0$. Since the pressure derivative of the Gibbs energy determines the sample volume, $V_{\rm s,n} = \partial G_{\rm s,n}/\partial p$, one finds $V_{\rm s} = V_{\rm n} - V\,\partial\varepsilon_{\rm con}/\partial p$, i.e., $\alpha = \partial\varepsilon_{\rm con}/\partial p$. This relation allows us to show that the force $\mathbf{F}_{\rm Sim}$ from (2) equals the electrostatic force caused by the second term of the

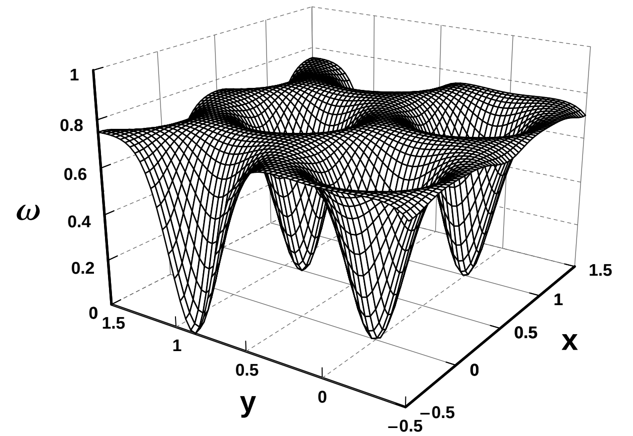

FIG. 1: The superconducting fraction $\omega = 2|\psi|^2/n$ in the triangular Abrikosov vortex lattice. We assume niobium with the GL parameter increased by non-magnetic impurities to $\kappa = 1.5$, the temperature $T = 0.7\,T_{\rm c}$ and the mean magnetic field $\bar B = 0.24\,B_{\rm c2}$. In centers of vortices the superconducting fraction ω goes to zero, while between vortices it approaches its non-magnetic value $1 - T^4/T_{\rm c}^4 = 0.76$.

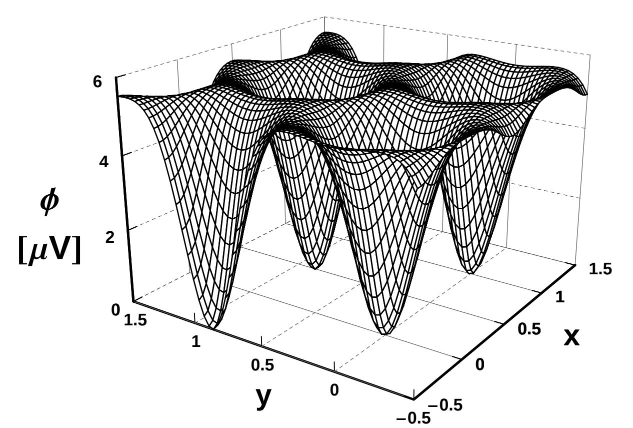

FIG. 2: The electrostatic potential for the parameters of Fig. 1. Its shape reminds the superconducting fraction shown in Fig. 1, which indicates that corrections beyond the approximation of Khomskii and Kusmartsev are small.

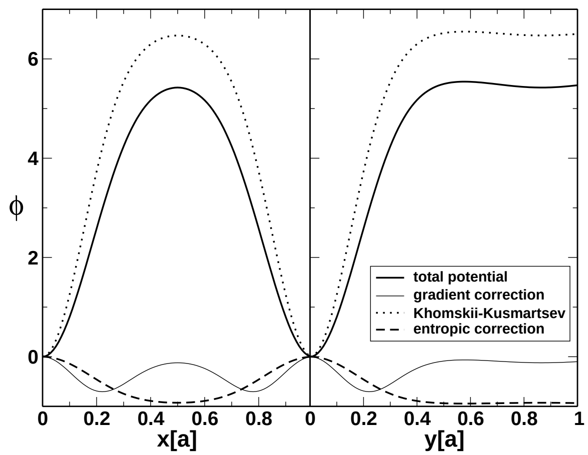

FIG. 3: Cuts through the electrostatic potential from Fig. 2. The thick full line represents the total potential (4), the dot line is the Khomskii-Kusmartsev approximation. The thin full line is the gradient correction given by the 'kinetic energy' term of (4), and the dashed line is the entropic correction given by the last term of (4).

Bernoulli potential (4).

To proceed, we will use the fact that the pressure modifies the condensation energy indirectly by an increase of the electron density

$$\alpha = \frac{\partial \varepsilon_{\rm con}}{\partial p} = \frac{\partial \varepsilon_{\rm con}}{\partial n}\frac{\partial n}{\partial p} = \frac{\partial \varepsilon_{\rm con}}{\partial n}\frac{n}{K}. \tag{5}$$

In the rearrangement we have employed the definition of the bulk modulus $K = -V/(\partial V/\partial p) = n/(\partial n/\partial p)$. Substituting (5) into the force (2) one finds

$$\mathbf{F}_{\rm Sim} = n\,\frac{\partial \varepsilon_{\rm con}}{\partial n}\,\nabla\frac{2|\psi|^2}{n}. \tag{6}$$

Comparing (6) with (3) one can see that the force introduced by Šimánek equals to the electrostatic force due to the second term of the Bernoulli potential (4). In this sense, the approximation used within the theory of deformable superconductors is equivalent to the approximation of the electrostatic potential derived by Khomskii and Kusmartsev. The gradient and entropic corrections of the Bernoulli potential (4) provide us with corresponding corrections to the force of Šimánek.

More interesting is the gradient correction. From the formula (4) follows that far from the vortex core, where $\bar\psi\psi \to (1-T^4/T_{\rm c}^4)\,n/2$, the gradient correction is proportional to the square of the local current. For an isolated vortex, the gradient correction thus decays on the scale of the London penetration depth. Consequently one can expect, that it plays an important role in high κ materials.

The effect of the gradient correction is traceable also for a conventional material assumed here. To be specific, our sample is a niobium rod parallel to the magnetic field. The GL coherence length of niobium is reduced by non-magnetic impurities so that the GL parameter is increased to $\kappa = 1.5$, while other material parameters remain close to values of the pure niobium. All plots are for $T = 0.7\,T_{\rm c}$ and $\bar B = 0.24\,B_{\rm c2}$. In this case the magnetic field is not split into separated unitary fluxes but it is nearly homogeneous with amplitude fluctuations of about 20% around the mean field $\bar B$. The vortex cores are well separated, however, as ω reaches its non-magnetic value in the out-of-core region, see Fig. 1.

Let us analyze the three contributions to the electrostatic potential from the point of view of forces they cause. According to the position of the inflex point of the Khomskii-Kusmartsev potential seen in Fig. 3, one can estimate that the maximum of the Šimánek force is at about $x, y \sim 0.1\,a$. This is quite close to the center of the vortex core. The gradient correction oscillates fast in space having a magnitude much smaller than the Khomskii-Kusmartsev potential. Its gradient, however, is rather comparable to the gradient of the dominant term, which shows that gradient contribution to the force can appreciably modify the Šimánek force. In the heart of the vortex core, the gradient correction to the force acts against the Šimánek force, while in the skin of the vortex core it points in the same direction. As a result, the maximum of the total force is shifted outwards to $x, y \sim 0.2\,a$.

Naturally, gradient corrections modify the vortex mass. Figure 4a shows how individual regions in the Abrikosov vortex lattice contribute to the vortex mass for the Šimánek force, in figure 4b the gradient and the entropic corrections are included. The plotted function is the density of kinetic energy of lattice ions driven by vortices moving with velocity V in the x direction [14]

$$E_{\rm kin} = \frac{1}{2}V^2\,n\,M\left[\left(\frac{\partial u_x}{\partial x}\right)^2 + \left(\frac{\partial u_y}{\partial x}\right)^2\right], \tag{7}$$

where M is the mass of a single ion.

In most places of the Abrikosov vortex lattice, the ionic kinetic energy is lowered by the correction terms, see Fig. 4. From the integral over the elementary cell one obtains the vortex mass per unit length. Keeping both corrections, the ion contribution to the vortex mass is reduced by a factor 0.83 as compared to Šimánek result. If one neglects the gradient correction keeping only the entropic correction, the reduction factor is 0.70. The gradient correction thus leads to a small enhancement of the vortex mass.

Comparing relative amplitudes of the kinetic energy inside and between the cores, one can see that the corrections have increased the share of the out-of-core region. Since the entropy term merely reduces the amplitude of the Šimánek force, this redistribution of distortions is exclusively due to the gradient correction. According to Cano, Levanyuk and Minyukov [19] the out-of-core lat-

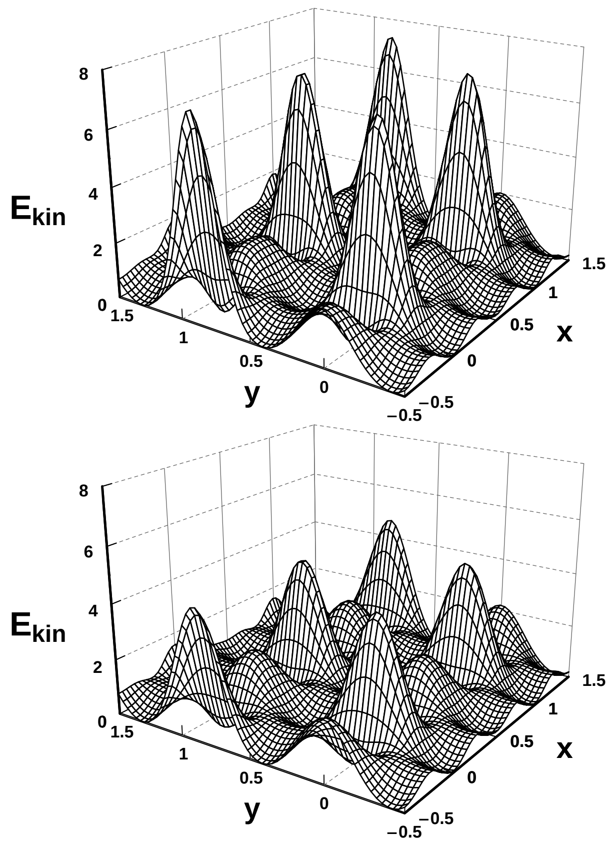

FIG. 4: The density of kinetic energy of lattice ions created by vortices moving in the x direction for parameters of Fig. 1. The kinetic energy due to (a) Šimánek force (6) , and (b) the electrostatic force (3). The plotted function is dimensionless a quantity identical to the bracket from the formula (7).

tice deformations are important for the strain-mediated interaction of vortices. We suggest that the theory of this interaction should be reexamined with the gradient correction included.

In summary, we have expressed the forces deforming a lattice of a superconductor in terms of the electrostatic force. This approach allows one to benefit from experiences accumulated within the theory of the so called Bernoulli potential. One directly obtains the gradient corrections we have discussed in this paper. We suggest that the theory of vortex motion should be revised taking this gradient corrections into account. The present theory is restricted to homogeneous isotropic materials. Its extension to layered materials we plan to discuss in short future.

This work was supported by research plans MSM 0021620834 and No. AVOZ10100521, by grants GAČR 202/04/0585 and 202/05/0173, and by European ESF program AQDJJ.

[1] D. Shoenberg, *Elements of Classical Thermodynamics* (Cambridge University Press, London 1961).
[2] R. R. Hake, Phys. Rev. **144**, 471 (1968).
[3] B. Obst, Phys. Stat. Sol. (b) **45**, 467 (1971).
[4] J. Schelten, Ft. Ullrnaier and W. Schmatz, Phys. Stat. Sol. (b) **48**, 649 (1971).
[5] U. Essmann, Physica **55**, 83 (1971).
[6] H. Weber, J. Schelton, and G. Lippmann, Phys. Stat. Sol. (b) **57**, 515 (1973).
[7] R. Ullmaier, R. Zeller and P. H. Dederichs, Phys. Lett. A **44**, 331 (1973).
[8] L. J. Campbell, M. M. Doria and V. G. Kogan, Phys. Rev. B **38**, 2439 (1988).
[9] H. F. Hess, C. A. Murray and J. V. Waszczak, Phys. Rev. Lett. **69**, 2138 (1992).
[10] H. F. Hess, C. A. Murray and J. V. Waszczak, Phys. Rev. B **50**, 16528 (1994).
[11] C. A. Bolle, F. DeLaCruz, P. L. Gammel, J. V. Waszczak and D. J. Bishop, Phys. Rev. Lett. **71**, 4039 (1993).
[12] P. L. Gammel, D. A. Huse, R. N. Kleiman, B. Batlogg, C. S. Oglesby, E. Bucher, D. J. Bishop, T. E. Mason and K. Mortensen, Phys. Rev. Lett. **72**, 278 (1994).
[13] V. G. Kogan, L. N. Bulaevskii, P. Miranović and L. Dobrosavljević-Grujić, Phys. Rev. B **51**, 15344 (1995).
[14] E. Šimánek, Phys. Lett. A **154**, 309 (1991).
[15] J.-M. Duan and E. Šimánek, Phys. Lett. A **190**, 118 (1992).
[16] M. W. Coffey, Phys. Rev. B **49**, 9774 (1994).
[17] E. M. Chudnovsky and A. B. Kuklov, Phys. Rev. Lett. **91**, 067004 (2003).
[18] H. Svensmark and L. M. Falicov, Phys. Rev. B **40**, 201 (1989).
[19] A. Cano, A. P. Levanyuk and S. A. Minyukov, Phys. Rev. B **68**, 144515 (2003).
[20] E. J. Kramer and C. L. Bauer, Philos. Mag. **15**, 1189 (1967).
[21] R. Labusch, Phys. Rev. **170**, 470 (1968).
[22] L. D. Landau and E. M. Lifshitz, *Elasticity* (Pergamon, Oxford, 1975).
[23] U. Kammerer, Z. Physik **227**, 125 (1969).
[24] F. London, *Superfluids* (Willey, New York, 1950), Vol. I, Sec. 8.
[25] A. G. van Vijfeijken and F. S. Staas, Phys. Lett. **12**, 175 (1964).
[26] D. I. Khomskii and F. V. Kusmartsev, Phys. Rev. B **46**, 14245 (1992).
[27] P. Lipavský, J. Koláček, K. Morawetz and E. H. Brandt, Phys. Rev. B **65**, 144511 (2002).
[28] T. H. Johansen, J. Lothe and H. Bratsberg, Phys. Rev. Lett. **80**, 4757 (1998).